

Scope of Work
(B. C. Gibb, Tulane University)

Prof Bruce Gibb will act as co-Investigator for this R01 application with Dr. David Mobley, Contact PI, from the University of California, Irvine. The specific subcontract work that Prof. Gibb will perform at Tulane University is detailed in Specific Aim 2. This work includes the synthesis of three deep-cavity cavitand hosts possessing different shaped binding pockets and water-solubilizing coats. We will utilize Isothermal Titration Calorimetry (ITC), and where necessary companion NMR studies, to determine the thermodynamics of guest binding to these different hosts. The work will provide blinded datasets to allow computational chemists to refine their methods for ascertaining the thermodynamics of complexation. Each set of experiments performed will possess a unique set of independent variables to probe specific questions pertaining to the Hydrophobic and Hofmeister effects, and ensure that the complete series of predictive challenges will not be biased in favor of or against any particular computational technique.